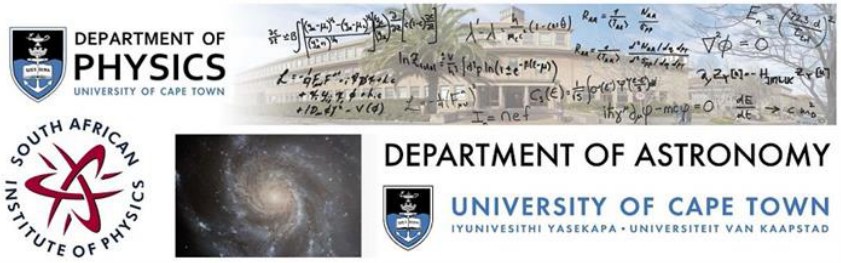

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Phase Stability Study of Nickel Doped Spinel LiMn₂ O₄ Using Cluster Expansion Method

Tuesday, 5 July 2016 16:10 (1h 50m)

Abstract content
   (Max 300 words)
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One of the challenges for improving the performance of lithium-ion batteries to meet increasingly demanding requirements for energy storage is the development of suitable cathode materials. Spinel-structured LiMn₂ O₄(LMO) is a desirable cathode material for Li-ion batteries, due to its low cost, abundance and high power capability. However, LMO suffers from limited cycle life that is triggered by manganese dissolution into the electrolyte during electrochemical cycling. Doping in battery materials tends to improve the efficiency in maintaining electrochemical capacity over a large number of cycles without sacrificing initial reversible capacity at room temperature. In this paper, Universal Cluster Expansion (UNCLE) code implemented in cluster expansion formalism is used to investigate nickel doped LMO phase stabilities. The method determines stable multi-component crystal structures and rank metastable structures by enthalpy of formation, while maintaining the predictive power and accuracy of first-principles density functional methods. Complex configurations of nickel doped LMO systems with various concentrations are determined at different temperatures by means of Monte Carlo random sampling. The ground state phase diagram generated various structures with different concentrations and symmetries. The findings predict that nickel doped LMO with 50:50 concentration of manganese and nickel is the most stable phase.

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